**Homework 3**

1. A porous spherical polymer of radius *R* contains a drug used to treat brain tumors. Experiments were performed *in vitro* to characterize the release of the drug. At the surface of the polymer sphere (i.e., ), the drug concentration is . Far from the surface of the polymer, the drug concentration drops to zero. **(A)** Derive an expression for the concentration profile for a radial position . **(B)** Derive an expression for determining the flux of the drug at the polymer surface. ***(Ans: part B = )***

**Ans:**

Part A: Deriving the Concentration Profile

The full mass transport equation in spherical coordinates is:

Assumptions:

Steady-state:

No convection:

Spherical symmetry: no dependence on

No generation or consumption:

Equation simplifies to:

Step 3: Solve the Differential Equation

First integration:

Dividing by and integrate again:

Applying boundary conditions:

and

Part B: determining flux at the surface

Useing Fick’s first law:

Differentiate:

At

1. Consider steady 1D diffusion through a funnel of varying cross section as shown below. Unlike a straight tube with constant cross-section, the concentration varies nonlinearly with distance. Assume that no convection or chemical reactions occur in the control volume. The radius of the funnel can be modeled as:

Assume the concentration at is and the concentration at is . **(A)** Derive an expression for the concentration profile in this volume. **(B)** Derive an expression for the solute flux . **(C)** Determine the mass transfer coefficient for this system. Hint: A mass balance would show that for all values of . Another hint: Don’t jump straight into Fick’s Second Law; rather, rederive Fick’s Second Law (like we did in class) accounting for the change in areas in our control volume.

**(Ans: part C = )**

**Ans:**

Part A: concentration profile derivation

Mass balance for steady-state, no reaction scenario:

Relating Flux and Concentration using Fick’s first law

Thus:

Integrating once:

Solving for

Integrating again to find

Applying boundary conditions and

Complete concentration profile:

Part B: Solute flux derivation

Using Fick's first law:

Substitute the derived concentration profile:

Part C:

Mass transfer coefficient relates flux and concentration difference:

Comparing with previous flux expression:

By canceling

1. The diffusion of a protein into tissue is studied at short times by measuring the uptake of the labeled protein into the tissue of thickness *L*. Initially there is no labeled protein in the tissue layer. At time zero, the surface at has a (constant) concentration of . **(A)** Assuming the tissue can be modeled as a semi-infinite medium, derive an expression for the protein concentration profile as a function of both time and position. **(B)** Derive an expression for determining the protein uptake which can be defined as:

Given the following values for the system:

(where is the area normal to the direction of protein movement), **(C)** determine the value for the diffusion coefficient. **(D)** Use the diffusion coefficient found in part C and the given time window () and tissue thickness to validate the assumption of a semi-infinite medium. Determine the approximate time when the model’s assumption may no longer be valid (defined when the concentration of the protein at the far edge of the tissue is 1% of ). **(Ans: part C = ; part D = )**

**Ans**:

Part A: Deriving the Protein Concentration Profile

Assuming no convection and reaction, using Fick’s second law:

Boundary Conditions:

The solution is free of solute at the beginning

Constant surface concentration

Semi-infinite medium

The concentration profile is given by the complementary error function (erfc):

Part B: Deriving Protein Uptake

Flux calculation using Fick’s First Law:

Integrate flux for uptake:

Part C: Calculating the Diffusion Coefficient

Given,

Rearrange Uptake Equation

Part D: Validating the Semi-Infinite Assumption

Boundary Layer Thickness at :

Since , which is greater than boundary layer thickness at 600 s, the assumption is valid.

Time When Model Fails:

1. A solid sphere with diameter 2 mm has a thin film of a drug (with diffusion coefficient ) coated on its surface. Water at 37 °C (kinematic viscosity ) flows past the sphere with an average velocity of 2 cm/s. Assume the drug concentration far from the surface of the sphere is zero. **(A)** Determine the Reynolds, Schmidt, and Sherwood numbers for this system. **(B)** Calculate the mass transfer coefficient .**(Ans: part B = )**

**Ans:**

Part A: Determination of Dimensionless Numbers

Reynolds number characterizes fluid flow (ratio of inertial to viscous forces):

The Schmidt number characterizes momentum diffusivity (viscosity) versus mass diffusivity:

Sherwood number characterizes convective mass transport compared to diffusion:

Part B: mass transfer coefficient

The Sherwood number can also be expressed as a relationship to the mass transfer coefficient:

Solve for kmk\_m:

km=Sh⋅Ddk\_m = \frac{Sh \cdot D}{d}

Plugging in known values:

* Sh=48.33Sh = 48.33
* D=6.3×10−6 cm2/sD = 6.3 \times 10^{-6}\,\text{cm}^2/\text{s}
* d=0.2 cmd = 0.2\,\text{cm}

Thus:

km=(48.33)(6.3×10−6 cm2s)0.2 cmk\_m = \frac{(48.33)(6.3 \times 10^{-6}\,\frac{\text{cm}^2}{\text{s}})}{0.2\,\text{cm}}

Compute step-by-step:

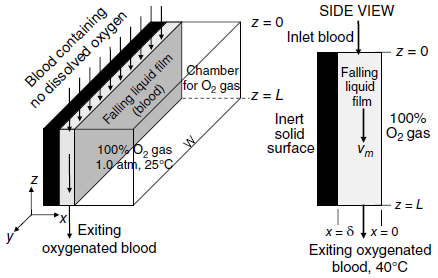
* Numerator: 48.33×6.3×10−6=3.04479×10−448.33 \times 6.3 \times 10^{-6} = 3.04479 \times 10^{-4}
* Denominator: 0.20.2

Hence:

km=3.04479×10−40.2=1.522×10−3 cmsk\_m = \frac{3.04479 \times 10^{-4}}{0.2} = 1.522 \times 10^{-3}\,\frac{\text{cm}}{\text{s}}

asfd

1. A device has been proposed that will serve as a blood oxygenator for a heart-lung bypass machine. In this process, deoxygenated blood enters the top of the chamber and falls down as a liquid film of uniform thickness. Contacting the liquid surface is pure oxygen gas. Assume that the width of the liquid film () is much larger than the length . Assume the velocity of the falling blood film is uniform. Assume the concentration of oxygen in the blood at its surface in contact with the oxygen gas can be modeled with Henry’s Law. Assume the thickness of the blood film is thick enough that we can modeled the blood as a semi-infinite medium. **(A)** Derive an expression for the concentration profile of oxygen within the blood as a function of *x* and *z* (your expression should also include the pressure of the oxygen gas , the Henry’s constant for the gas , the diffusion coefficient for oxygen in blood , and the average uniform velocity of the blood ). **(B)** Calculate the diffusion coefficient for oxygen in blood using the Stokes-Einstein equation; assume the blood has a temperature of 40oC and a dynamic viscosity of 3.5 cP. **(C)** It is noted that the thickness of the blood film is and the length over which oxygen diffuses into the blood is . Determine the minimum flow rate (per unit width) of blood that enters the oxygenator such that the assumption of treating the blood as a semi-infinite medium. (Hint: the assumption will be satisfied if the film thickness is equal to or larger than the concentration boundary layer). **(Ans: part C = )**



**Ans:**